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Canonical Runge–Kutta–Nyström methods of orders five and six ☆

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Abstract

In this paper, we construct canonical explicit five-stage and seven-stage Runge–Kutta–Nyström methods of orders five and six, respectively, for Hamiltonian dynamical systems.

Keywords: Hamiltonian systems; Canonical integrators: Symplectic integrators; Runge–Kutta–Nyström methods

1. Introduction

There has been much recent interest in deriving for Hamiltonian systems

$$\frac{dq}{dt} = \frac{\partial H(q, p)}{\partial p}, \qquad \frac{dp}{dt} = -\frac{\partial H(q, p)}{\partial q}, \tag{1}$$

higher-order numerical integrators which retain the canonical (or symplectic) property of the flow of the original system. Of particular interest have been explicit Runge–Kutta–Nyström (RKN) methods for the special separable Hamiltonian

$$H(q, p) = \tfrac{1}{2} p^{\mathrm{T}} M^{-1} p + V(q), \tag{2}$$

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where q and p are vectors representing, respectively, the positions and momenta and where M is a diagonal matrix. The function $V(q)$ is associated with the potential energy and H with the total energy.

Ruth [9] was the first to publish results about canonical numerical integrators. He showed that the second-order one-stage leapfrog–Störmer–Verlet method was canonical and discovered three-stage canonical RKN method of order three. Ruth's work was followed by considerable research in the area of constructing higher-order canonical integrators, [2,3,6,10–12]. Forest and Ruth [3] derived an explicit three-stage canonical integrator of order four. Yoshida [12] was the first to prove the existence of canonical integrators of arbitrarily high order. He showed how to construct a 3^k-stage method having order $2k+2$ using a composition of canonical one-stage methods of order two. He derived numerically seven- and fifteen-stage canonical integrators, respectively of orders six and eight, using a Lie group approach. Low stage number is desirable because of greater convenience (such as the generation of more closely spaced output values).

Still much is unknown about the possibilities for higher-order canonical methods — information that is useful in the search for practical methods. In this paper we derive numerically fifth-order, five-stage RKN methods and symmetric sixth-order, seven-stage RKN methods in Section 3. A total of four fifth-order, five-stage RKN methods are reported. Sixteen symmetric sixth-order, seven-stage RKN methods were obtained, three of these are equivalent (in the sense used in [6]) to the canonical integrators constructed in [12] for general separable Hamiltonians.

2. Order and canonical conditions

An s-stage Runge–Kutta–Nyström method for a system with the Hamiltonian (2) is given by

$$\begin{aligned} y_i &= q_n + c_i h\dot{q}_n + h^2 \sum_{j=1}^{s} a_{ij} f(y_j), \quad i = 1, 2, \ldots, s, \\ q_{n+1} &= q_n + h\dot{q}_n + h^2 \sum_{i=1}^{s} b_i f(y_i), \quad \dot{q}_{n+1} = \dot{q}_n + h \sum_{i=1}^{s} B_i f(y_i), \end{aligned} \tag{3}$$

where $\dot{q}_n = M^{-1} p_n$ and $f(q) = -M^{-1}\ \nabla V(q)$. Method (3) is explicit if $a_{ij} = 0$ for $j \geqslant i$. An explicit s-stage RKN method without redundant stages is canonical if [6,7,11]

$$b_i = B_i(1 - c_i), \qquad 1 \leqslant i \leqslant s, \tag{4}$$

$$a_{ij} = B_j(c_i - c_j), \quad j < i. \tag{5}$$

If we assume that the conditions in (4) and (5) are satisfied, we have [4] the following order conditions for RKN methods of order $\leqslant 5$:

t_1: $\sum_i B_i = 1$,

t_2: $\sum_i B_i c_i = \frac{1}{2}$,

t_3: $\sum_i B_i c_i^2 = \frac{1}{3}$,

t_4: $\sum_i \sum_{j<i} B_i B_j (c_i - c_j) = \frac{1}{6}$,

t_5: $\sum_i B_i c_i^3 = \frac{1}{4}$,

t_6: $\sum_i \sum_{j<i} B_i B_j c_i (c_i - c_j) = \frac{1}{8}$,

t_7: $\sum_i \sum_{j<i} B_i B_j (c_i - c_j) c_j = \frac{1}{24}$,

t_8: $\sum_i B_i c_i^4 = \frac{1}{5}$,

t_9: $\sum_i \sum_{j<i} B_i B_j c_i^2 (c_i - c_j) = \frac{1}{10}$,

t_{10}: $\sum_i \sum_{j<i} \sum_{l<i} B_i B_j B_l (c_i - c_j)(c_i - c_l) = \frac{1}{20}$,

t_{11}: $\sum_i \sum_{j<i} B_i B_j c_i c_j (c_i - c_j) = \frac{1}{30}$,

t_{12}: $\sum_i \sum_{j<i} B_i B_j c_j^2 (c_i - c_j) = \frac{1}{60}$,

t_{13}: $\sum_i \sum_{j<i} \sum_{l<j} B_i B_j B_l (c_i - c_j)(c_j - c_l) = \frac{1}{120}$.

The condition t_7 is redundant (see [6]). We use a similar approach as in [6] to show that t_{12} and t_{13} are also redundant:

$$
\begin{aligned}
\text{left-hand side of } t_{12} &= \sum_i \sum_{j<i} B_i B_j c_j^2 (c_i - c_j) = -\sum_i \sum_{j>i} B_i B_j c_i^2 (c_i - c_j) \\
&= \sum_i \sum_{j<i} B_i B_j c_i^2 (c_i - c_j) - \sum_i \sum_j B_i B_j c_i^2 (c_i - c_j) \\
&= \tfrac{1}{10} - \left(\sum_i \sum_j B_i B_j c_i^3 - \sum_j \sum_i B_i B_j c_i^2 \right) \\
&= \tfrac{1}{10} - \left(\tfrac{1}{4} \cdot 1 - \tfrac{1}{3} \cdot \tfrac{1}{2} \right), \\
&= \tfrac{1}{60} = \text{right-hand side of } t_{12}, \\
\text{left-hand side of } t_{13} &= \sum_i \sum_{j<i} \sum_{l<j} B_i B_j B_l (c_i - c_j)(c_j - c_l) \\
&= -\sum_i \sum_{j>i} \sum_{l<i} B_i B_j B_l (c_i - c_j)(c_i - c_l) \\
&= \sum_i \sum_{j<i} \sum_{l<i} B_i B_j B_l (c_i - c_j)(c_i - c_l) - \sum_i \sum_j \sum_{l<i} B_i B_j B_l (c_i - c_j)(c_i - c_l) \\
&= \tfrac{1}{20} - \sum_j B_j \left[\sum_i \sum_{l<i} B_i B_l (c_i - c_l) c_i - \sum_i \sum_{l<i} B_i B_l (c_i - c_l) c_j \right] \\
&= \tfrac{1}{20} - \left[1 \cdot \tfrac{1}{8} - \sum_j B_j c_j \sum_l \sum_{l<i} B_i B_l (c_i - c_l) \right] \\
&= \tfrac{1}{20} - \left(1 \cdot \tfrac{1}{8} - \tfrac{1}{2} \cdot \tfrac{1}{6} \right) = \tfrac{1}{120} = \text{right-hand side of } t_{13}.
\end{aligned}
$$

The above results illustrate the proposition of [1] that states that if two Nyström trees are equivalent (see the definition in the Appendix), then the Φ (see the Appendix) that corresponds to one can be expressed in terms of Φ's of the other and trees of lower orders. In our case, the trees $f[z^2, f]$ and $f[f[z^2]]$ in our special notation (see the Appendix) that result, respectively, from t_9 and t_{12} are equivalent. The same is true for trees $f[f[z]^2]$ and $f[f[f]]$ that result, respectively, from t_{10} and t_{13}.

3. Canonical Runge–Kutta–Nyström methods

3.1. Fifth-order five-stage methods

In Section 2, we showed that t_7, t_{12} and t_{13} are redundant for a canonical RKN method of fifth order, leaving us with ten conditions involving ten parameters. These conditions were then solved for B_i and c_i. We resorted to an iterative procedure because these conditions involve complicated expressions in B_i and c_i. We used the subroutines HYBRD1 and HYBRJ1 of MINPACK obtained from Netlib for determining the solution. HYBRD1 combines Powell's method for optimization, QR factorization and the finite divided difference method for computing the Jacobian matrix. HYBRJ1 is the same as HYBRD1, except that an exact Jacobian matrix is used. The initial guesses were obtained randomly from a Gaussian distribu-

Table 1
Fifth-order five-stage Runge–Kutta–Nyström methods

Method	B_i	c_i
1	−1.670 808 923 273 143 120 60	0.694 913 891 070 179 312 59
	1.221 439 092 309 975 382 70	0.637 071 996 769 983 384 11
	0.088 495 158 132 539 081 25	−0.020 557 569 982 115 980 05
	0.959 970 880 137 701 598 76	0.795 861 896 345 753 550 01
	0.400 903 792 692 977 933 85	0.301 166 242 723 777 788 37
2	0.221 161 934 424 179 029 70	0.770 703 449 439 395 393 84
	1.002 184 715 210 517 662 60	0.245 641 664 783 706 747 95
	0.204 202 868 930 455 389 01	0.872 951 015 566 575 838 63
	−0.824 377 563 595 430 684 63	0.133 524 180 174 383 666 49
	0.396 828 045 030 280 518 46	0.038 270 099 854 273 660 62
3	0.400 903 792 696 647 776 06	0.698 833 757 275 446 942 89
	0.959 970 880 134 123 905 06	0.204 138 103 654 598 890 29
	0.088 495 158 127 216 339 01	1.020 557 570 004 185 343 70
	1.221 439 092 349 102 528 70	0.362 928 003 230 752 915 80
	−1.670 808 923 307 090 410 00	0.305 086 108 931 675 648 04
4	0.396 828 045 027 481 202 12	0.961 729 900 146 376 492 92
	−0.824 377 563 590 000 805 86	0.866 475 819 826 055 260 19
	0.204 202 868 931 428 999 09	0.127 048 984 433 927 286 69
	1.002 184 715 207 946 164 00	0.754 358 335 216 376 407 75
	0.221 161 934 423 144 329 60	0.229 296 550 560 405 959 51

tion with mean 0 and standard deviation 1. About 10000 different initial guesses were tried and only four methods were obtained. These four methods, obtained using HYBRD1, were used as initial solutions for the HYBRJ1 program to improve the accuracy of method coefficients. These four methods are shown in Table 1. The two-norm of residuals in all thirteen order conditions is 10^{-13} for Method 1, 10^{-14} for Methods 2, 10^{-15} for Methods 3 and 4. As is obvious, Method 3 is the adjoint of Method 1, and Method 4 the adjoint of Method 2. The adjoint of a method is obtained by interchanging h, q_n and $\dot{q}_n$, respectively, with $-h$, q_{n+1} and $\dot{q}_{n+1}$. The slight differences in coefficients indicate the error in these values. We speculate that these are the only methods with real coefficients considering the magnitude of the number of initial guesses tried. Very recently, we also found these methods in [8].

3.2. Sixth-order six-stage methods

To construct symmetric methods of order six, we start with a six-stage RKN method with the following conditions:

$$B_1 = B_6, \qquad B_2 = B_5, \qquad B_3 = B_4,$$
$$c_1 = 1 - c_6, \qquad c_2 = 1 - c_5, \qquad c_3 = 1 - c_4.$$

With these conditions, t_1, t_3, t_4 and t_8 can be written as

$$t_1: \quad B_4 + B_5 + B_6 = \tfrac{1}{2},$$
$$t_3: \quad B_4 c_4(1 - c_4) + B_5 c_5(1 - c_5) + B_6 c_6(1 - c_6) = \tfrac{1}{12},$$
$$t_4: \quad B_5 c_5(B_4 + B_5) + B_6 c_6(1 - B_6) + B_4(B_4 c_4 + B_5 c_5) = \tfrac{5}{24},$$
$$t_8: \quad B_4 c_4^2(1 - c_4)^2 + B_5 c_5^2(1 - c_5)^2 + B_6 c_6^2(1 - c_6)^2 = \tfrac{1}{60}.$$

The conditions t_2, t_5 and t_6 are redundant given t_1, t_3, t_4 and the symmetry conditions. For details, see [5]. The conditions t_9, t_{10} and t_{11} have complicated expressions, even after they have been simplified; they are omitted here. For a symmetric six-stage RKN method, it turns out that t_1, t_3, t_4, t_8 and two of t_9, t_{10}, t_{11} are enough to find B_4, B_5, B_6, c_4, c_5 and c_6. In all, there are three possible sets of equations, namely,

$$t_1, t_3, t_4, t_8, t_9, t_{10}, \qquad t_1, t_3, t_4, t_8, t_9, t_{11}, \qquad t_1, t_3, t_4, t_8, t_{10}, t_{11}.$$

The three sets were solved by HYBRD1 and all solutions obtained from each set never satisfied the missing equation after trying 1000 initial guesses. We therefore state the following conjecture.

Conjecture 1. *There is no symmetric six-stage RKN method of order six.*

3.3. Sixth-order seven-stage methods

The negative result above motivated us to search for symmetric seven-stage methods of order six. The symmetry conditions in this case are

$$B_1 = B_7, \qquad B_2 = B_6, \qquad B_3 = B_5,$$
$$c_1 = 1 - c_7, \qquad c_2 = 1 - c_6, \qquad c_3 = 1 - c_5, \qquad c_4 = \tfrac{1}{2}.$$

Table 2
Sixth-order seven-stage Runge–Kutta–Nyström methods

	Method 1 (10^{-18})	Method 2 (10^{-11})	Method 3 (10^{-10})	Method 4 (10^{-13})
B_4	0.269 875 771 871 336 403 73	3.592 860 744 352 452 464 4	0.000 242 860 409 775 017 24	0.050 519 380 394 960 374 00
$B_5 = B_3$	0.921 619 775 048 851 893 58	−15.107 332 703 974 111 123 0	0.081 913 850 070 433 720 04	−0.197 242 961 898 152 507 92
$B_6 = B_2$	0.131 182 410 201 052 806 26	12.863 477 709 969 692 675 0	−0.231 586 422 482 352 842 81	0.294 213 837 109 505 942 04
$B_7 = B_1$	−0.687 740 071 185 572 901 71	0.947 424 621 828 192 215 9	0.649 551 142 207 031 614 14	0.377 769 434 591 166 378 88
c_4	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 0	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 00
$c_5 = 1 - c_3$	0.065 208 629 876 803 410 24	0.618 374 874 392 089 766 2	1.435 313 159 331 936 550 10	0.174 006 973 179 405 882 48
$c_6 = 1 - c_2$	0.653 737 694 837 447 789 01	0.615 797 157 767 439 752 3	−0.245 170 483 595 757 197 67	0.351 121 574 384 983 421 80
$c_7 = 1 - c_1$	0.055 866 078 117 873 765 72	0.207 832 884 810 862 442 0	0.889 616 733 536 844 935 04	0.885 384 505 851 166 391 29
	Method 5 (10^{-14})	Method 6 (10^{-14})	Method 7 (10^{-12})	Method 8 (10^{-12})
B_4	0.534 332 765 761 637 839 88	−1.175 515 920 851 519 885 40	0.009 322 186 739 771 197 32	1.831 158 710 434 821 159 80
$B_5 = B_3$	0.267 612 297 910 370 914 71	0.182 555 824 044 905 643 71	0.324 985 725 999 458 628 48	−1.608 931 783 915 053 171 50
$B_6 = B_2$	−0.110 492 899 848 635 242 18	0.904 377 903 536 061 924 25	−0.881 659 125 352 316 636 93	0.786 441 145 515 187 018 50
$B_7 = B_1$	0.075 714 219 057 445 407 53	0.000 824 232 844 792 374 73	0.010 520 123 059 829 724 10	0.406 911 283 182 455 573 16
c_4	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 00
$c_5 = 1 - c_3$	0.890 041 172 383 401 543 10	0.083 399 341 965 787 453 64	−0.484 599 392 491 707 229 86	0.642 818 763 871 381 234 13
$c_6 = 1 - c_2$	0.386 495 000 905 543 661 20	0.601 119 266 133 079 300 40	1.317 701 148 657 114 169 50	0.193 747 105 591 459 649 16
$c_7 = 1 - c_1$	0.322 786 969 526 560 124 56	−0.444 722 551 246 128 402 18	−0.048 172 227 547 237 893 32	0.457 836 323 217 853 441 25
	Method 9 (10^{-18})	Method 10 (10^{-11})	Method 11 (10^{-14})	Method 12 (10^{-10})
B_4	0.178 705 563 516 043 062 04	1.315 186 320 721 332 728 90	2.376 352 744 307 751 954 70	2.389 447 783 260 779 979 80
$B_5 = B_3$	−0.707 258 656 031 231 291 22	−1.177 679 984 196 724 865 20	−2.132 285 222 001 450 712 50	0.001 528 862 283 234 480 38
$B_6 = B_2$	0.521 546 038 768 186 458 04	0.235 573 213 367 892 324 63	0.004 260 681 870 792 276 08	−2.144 035 316 316 961 988 20
$B_7 = B_1$	0.596 359 835 505 023 302 16	0.784 513 610 468 166 176 11	1.439 848 167 976 782 459 10	1.447 782 562 403 337 517 90
c_4	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 00
$c_5 = 1 - c_3$	0.193 726 736 771 476 410 95	0.568 753 168 250 185 575 54	0.622 033 761 153 150 701 11	1.695 488 322 715 980 270 00
$c_6 = 1 - c_2$	0.122 813 639 093 977 272 25	0.097 699 782 845 606 744 93	−0.441 978 508 912 101 982 13	0.624 235 095 751 464 410 18
$c_7 = 1 - c_1$	0.738 104 052 905 065 906 52	0.607 743 194 758 781 243 35	0.280 075 916 011 608 460 49	0.276 108 718 801 228 858 76
	Method 13 (10^{-12})	Method 14 (10^{-16})	Method 15 (10^{-13})	Method 16 (10^{-12})
B_4	0.380 641 590 970 195 135 86	−1.172 410 291 060 975 473 50	−1.199 488 496 335 889 128 20	0.403 733 335 389 475 050 81
$B_5 = B_3$	0.689 137 411 862 809 252 74	0.000 862 710 114 629 165 79	0.185 734 781 666 566 587 57	0.008 838 140 047 978 500 15
$B_6 = B_2$	−0.379 624 214 274 416 218 93	0.182 789 540 999 773 721 97	0.004 558 884 160 487 742 29	0.693 125 122 487 708 761 97
$B_7 = B_1$	0.000 166 006 926 509 398 25	0.902 552 894 416 084 489 00	0.909 450 582 340 890 234 26	−0.403 829 930 230 424 787 52
c_4	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 00	0.500 000 000 000 000 000 00
$c_5 = 1 - c_3$	0.843 994 257 281 080 298 45	1.408 981 366 235 929 655 80	0.085 898 990 290 794 093 24	1.131 516 036 660 900 879 50
$c_6 = 1 - c_2$	0.825 658 405 185 433 836 52	0.082 185 108 932 481 825 80	1.129 945 079 636 090 898 10	0.835 510 909 652 475 614 60
$c_7 = 1 - c_1$	2.013 087 978 988 176 471 20	0.600 104 575 325 873 684 29	0.593 835 629 255 283 262 51	0.814 258 127 524 347 688 71

With these conditions t_1, t_3, t_4 and t_8 can now be written as

$$t_1:\quad \tfrac{1}{2}B_4 + B_5 + B_6 + B_7 = \tfrac{1}{2},$$

$$t_3:\quad \tfrac{1}{8}B_4 + B_5c_5(1-c_5) + B_6c_6(1-c_6) + B_7c_7(1-c_7) = \tfrac{1}{12},$$

$$t_4:\quad \tfrac{1}{8}B_4^2 + B_5c_5(B_4+B_5) + B_6c_6(1-B_6) + B_7c_7(1-B_7) - 2B_6B_7c_6 = \tfrac{5}{24},$$

$$t_8:\quad \tfrac{1}{16}B_4 + 2B_5c_5^2(1-c_5)^2 + 2B_6c_6^2(1-c_6)^2 + 2B_7c_7^2(1-c_7)^2 = \tfrac{1}{30}.$$

The unknowns in this case are B_4, B_5, B_6, B_7, c_5, c_6 and c_7. This makes it likely that the conditions t_1, t_3, t_4, t_8, t_9, t_{10} and t_{11} can be solved uniquely for those parameters. Again, we used the routine HYBRD1. After trying 1000 different initial guesses, we obtained sixteen different methods as indicated in Table 2. The numbers in brackets represent the two-norms of the residuals of all 23 order conditions. We did not use HYBRJ1 to improve the accuracy of method coefficients as we did in Section 3.1. The sixth-order conditions are given in the Appendix for verification purposes. These methods which include the methods constructed in [12] are seven-stage, all of order six, counterexamples to what is suggested in [1].

Acknowledgement

We thank Skip Thompson for helping us to obtain better accuracy for the method coefficients with the use of HYBRJ1 and an exact Jacobian matrix.

Appendix. Order-six conditions

Using the notation of [4], we have that an RKN method applied to a problem of the form $y'' = f(y)$ is of order p if and only if

$$\sum b_i\Phi_i(t) = \frac{1}{(\rho(t)+1)\gamma(t)},\quad \text{for Nyström trees with } \rho(t) \leqslant p-1, \tag{6}$$

$$\sum B_i\Phi_i(t) = \frac{1}{\gamma(t)},\quad \text{for Nyström trees with } \rho(t) \leqslant p, \tag{7}$$

where $\rho(t)$ is the order of the tree, $\gamma(t)$ is the density of the tree and $\Phi_i(t)$ corresponds to the elementary weight of the Nyström tree. If conditions (4) combine with (7), then conditions (6)

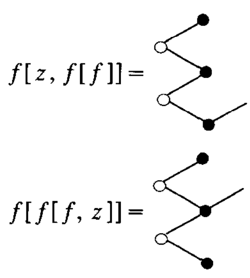

Fig. 1.

Table 3
Order-six conditions

t	$\rho(t)$	$\alpha(t)$	$\gamma(t)$	$\Phi_i(t)$
$f[z^5]$	6	1	6	c_i^5
$f[f^2, z]$	6	15	24	$\Sigma_j \Sigma_k a_{ij} a_{ik} c_i$
$f[f, z^3]$	6	10	12	$\Sigma_j a_{ij} c_i^3$
$f[z, f[f]]$ [a]	6	5	144	$\Sigma_j \Sigma_k a_{ij} a_{jk} c_i$
$f[f, f[z]]$	6	10	72	$\Sigma_j \Sigma_k a_{ij} a_{ik} c_k$
$f[z^2, f[z]]$	6	10	36	$\Sigma_j a_{ij} c_i^2 c_j$
$f[f[f, z]]$ [b]	6	3	240	$\Sigma_j \Sigma_k a_{ij} a_{jk} c_j$
$f[z, f[z^2]]$	6	5	72	$\Sigma_j a_{ij} c_i c_j^2$
$f[f[z^3]]$	6	1	120	$\Sigma_j a_{ij} c_j^3$
$f[f[f[z]]]$	6	1	720	$\Sigma_j \Sigma_k a_{ij} a_{jk} c_k$

are superfluous. Therefore, we concentrate on the conditions (7). First, we let $z = y'$ and then use a special notation (similar to what was used in our Mathematica program) to represent the trees or the elementary differentials. We give in Fig. 1 the correspondence between the elementary differentials in our notation and the Nyström trees for a few of the elementary differentials. The black node corresponds to the derivative of z and the white node to the derivative of the y. The bottom node is the root of the tree. Two Nyström trees are *equivalent* in the sense defined in [1], if they have equal number of black nodes, equal number of white nodes and identical branches and differ only in their roots. The order-six conditions are given in Table 3, where $\alpha(t)$ is the weight of the elementary differential.

References

[1] M.P. Calvo and J.M. Sanz-Serna, Order conditions for canonical Runge–Kutta–Nyström methods, *BIT* **32** (1992) 131–142.

[2] P.J. Channell and J.C. Scovel, Symplectic integration of Hamiltonian systems, *Nonlinearity* **3** (1990) 231–259.

[3] E. Forest and R.D. Ruth, Fourth-order symplectic integration, *Phys. D* **43** (1990) 105–117.

[4] E. Hairer, S.P. Nørsett and G. Wanner, *Solving Ordinary Differential Equations I: Non-Stiff Systems* (Springer, Berlin, 1987).

[5] D. Okunbor, Canonical integration methods for Hamiltonian systems, Ph.D. Thesis, Dept. Comput. Sci., Univ. Illinois, Urbana-Champaign, IL, 1992; Techn. Report UIUCD CS-R-92-1785.

[6] D. Okunbor and R.D. Skeel, Explicit canonical methods for Hamiltonian systems, *Math. Comp.* **59** (200) (1992) 439–455.

[7] D. Okunbor and R.D. Skeel, An explicit Runge–Kutta–Nyström method is canonical if and only if its adjoint is explicit, *SIAM J. Numer. Anal.* **29** (2) (1992) 521–527.

[8] M.-Z. Qin and W.-J. Zhu, Order conditions of two kinds of canonical difference schemes, *Comput. Math. Appl.* **25** (6) (1993) 61–74.

[9] R.D. Ruth, A canonical integration technique, *IEEE Trans. Nuclear Sci.* **NS-30** (4) (1983) 2669–2671.

[10] J.M. Sanz-Serna, The numerical integration of Hamiltonian systems, in: J.R. Cash and I. Gladwell, Eds., *Computational Ordinary Differential Equations* (Clarendon Press, Oxford, 1992) 437–449.

[11] Y.B. Suris, Canonical transformations generated by methods of Runge–Kutta type for the numerical integration of the system $x'' = -\partial U/\partial x$, *Zh. Vychisl. Mat. i Mat. Fiz.* **29** (1989) 202–211 (in Russian); also: *U.S.S.R. Comput. Math. and Math. Phys.* **29** (1) (1989) 138–144.

[12] H. Yoshida, Construction of higher order symplectic integrators, *Phys. Lett. A* **150** (1990) 262–268.